Discrete Ordinate Calculation of the k-Eigenvalue of an IFBA Pin Using Unstructured Meshes in 2D

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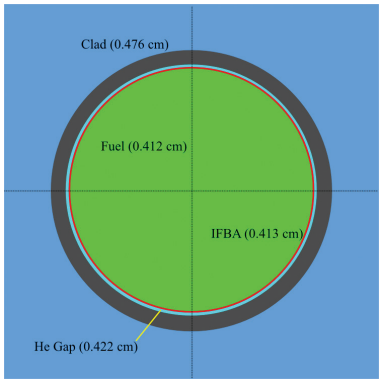
Integral Fuel Burnable Absorber (IFBA) pins are used for the reactivity control of the fuel assemblies of light water reactors. From the standpoint of the feasibility of performing a pin-resolved, 3D neutron transport computation of a full reactor core, the presence of IFBA pins represents a challenging problem. The traditional approach of homogenizing cross-sections inside the cells of a Cartesian mesh can be used to capture the neutronics effects associated with the thin IFBA coating via a discrete ordinate (SN) transport computation of the k-eigenvalue of the pin. Unfortunately, the number of spatial mesh cells required to resolve the thin neutron absorbing layer in a single pin can become prohibitively high, even in only 2D. We show how the use of unstructured meshes in the SN computation drastically reduces (100-fold reduction) the number of cells required to obtain the same k-eff, while eliminating recourse to cross-section homogenization.

Integral Fuel Burnable Absorber (IFBA) pins are used for the reactivity control of the uranium dioxide (UO_2) fuel assemblies of light water reactors [1]. IFBA is applied as a thin coating of zirconium diboride (ZrB_2) on the outer surface of the UO_2 pellets [2]. Specifically, the cross-sectional geometry of the IFBA pin is sketched in Fig. 1. The extension of the coolant box is equal to the standard 1.26-cm pin pitch of a 17×17 fuel assembly in a pressurized water reactor. Resolving the IFBA coating layer, only 0.001-cm thick, makes the transport problem particularly challenging. The pin's material composition is described in Table 1 and is loosely based on the specifications given in [1].

Table 1. Material composition of the IFBA pin.

Region	Density [g/cm^3]	Material
Fuel	10.24	UO_2 4.2%: U^{235}: 4.2 wt%, U^{238}: 95.8 wt%
IFBA	1.69	ZrB_2
Gap	0.001	O^{16}
Clad	6.504	Zircaloy-2: Zr/Sn/Fe/Cr/N= 98.23/1.50/0.12/0.10/0.05 at%
Coolant	1.0	H_20 at 293.125 K and 101.325 KPa

Fig. 1. Geometry specifications for the IFBA pin.



The k-eigenvalue (k-eff) calculation via the homogenization approach [3] was carried out using the PARTISN parallel neutral particle SN transport code. Specifically, we performed a convergence study for the k-eff by considering increasingly refined Cartesian meshes over a quarter of the pin with reflective boundary conditions. We utilized multi-group neutron cross-sections from the "mendf6" Nuclear Data Interface (NDI) library, for the 30-energy-group structure "30_LANL" [4]. A Legendre order of three was selected for the scattering expansion. The angular quadrature was the S8 square Chebychev-Legendre set, kept constant to focus on the differences between spatial mesh refinement for Cartesian and unstructured meshes. The results of the "spatial" convergence study are reported in Table 2.

Table 2. Spatial convergence of "homogenized" k-eff.

Spatial Mesh	k-eff
16×16	0.63850091
32×32	0.64022925
64×64	0.64068658
128×128	0.64091920
256×256	0.64108409
512×512	0.64118889
1024×1024	0.64125049
1152×1152	0.64125726
1280×1280	0.64126246
1408×1408	0.64126647
1536×1536	0.64126974

The refinement was arrested when convergence was achieved within 0.00001, obtaining a k-eff of 0.64127. This result was obtained for the 1408×1408 mesh consuming a solution time of 8998 seconds on 256 processors of the Typhoon cluster. The total number of sweeps was 13042 (58 outers).

We created a set of PYTHON scripts for the generation of unstructured meshes that cover either the entire pin, or just a hemisphere or a quarter. Each material region is subdivided into a set of radial and azimuthal intervals, used to generate an unstructured mesh whose origin is coincident with the pin's center. The radial sector closest to the origin is subdivided into triangular finite

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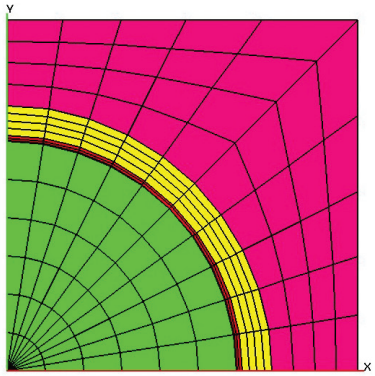

Fig. 2. A 17×10 unstructured mesh over a pin quarter.

elements. The remaining radial sectors are composed of quadrilaterals, to minimize the number of mesh cells. To fix ideas, a mesh example is given in Fig. 2.

The mesh in Fig. 2 is composed of 10 azimuthal intervals and 17 radial intervals: 6 in the fuel, 1 in the IFBA, 2 in the gap, 4 in the clad, and 4 in the coolant. Since no mesh cell contains more than one material, cross-section homogenization is not needed. The PYTHON scripts are also used to compute adjusted densities for the materials in the various regions of the meshed pin. This is done so that the mass of material in each meshed region is equal to the mass contained in the original curved volume for that region.

We used the CAPSAICIN parallel neutral particle SN code to compute the pin's k-eff over a fine unstructured mesh composed of 630 radial points: 412 in the fuel, 1 in the IFBA, 9 in the gap, 54 in the clad, and 154 in the coolant. The above choice results in a fine radial mesh where each radial interval is as thick as the radial extent of the IFBA coating. Using the same cross-section libraries and transport parameters as for the homogenization approach, we performed the azimuthal convergence study for the k-eff reported in Table 3.

Table 3. k-eff solution on a fine unstructured mesh.

Spatial mesh	k-eff
630×16	0.64130166
630×32	0.64128252
630×64	0.64127805
630×128	0.64127956
630×256	0.64128090

The converged k-eff is equal to 0.64128, and differs by 0.00001 from the "homogenized" value of 0.64127. The discrepancy stems from the fact that while CAPSAICIN exploits a bilinear discontinuous finite element method, PARTISN utilizes a linear discontinuous discretization.

We also investigated strategies for reducing the number of cells in the unstructured mesh computation. An encouraging result was obtained for a mesh composed of 228 radial intervals: 206 in the fuel, 2 in the IFBA, 4 in the gap, 8 in the clad, and 8 in the coolant. The k-eff was again 0.64128 and was already obtained for a 228×64 mesh, by switching from a linear to a logarithmically decreasing distribution of the radial points in the fuel, to appropriately resolve the transport effects near the fuel-IFBA interface. The computation took 1050 seconds on 240 processors. The total number of sweeps was 273, and a sweep includes all (30) energy groups. The above results were obtained exploiting CAPSAICIN's parallel decomposition in energy, using 30 energy processor groups. Finally, details on the non-linear formulation of the eigenvalue problem, and related solvers, used by the code can be found in [5]. The performance gain of the unstructured mesh strategy over the traditional homogenization approach is illustrated in Table 4.

Table 4. Performance of unstructured mesh approach.

	PARTISN	CAPSAICIN	Reduction Factor
Mesh cell count	1982464	14592	136
Solution time (seconds)	8998	1050	8.6
Sweep time (seconds)	0.69	0.13	5.3

The unstructured mesh calculation results in a 100-fold reduction in the number of mesh cells, consuming a solution time that is almost nine times lower than for the homogenization approach. We expect that the encouraging results obtained in 2D will favorably extend to higher dimensionality, and we will investigate the 3D case in our future research.

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